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13838-08-9 | DTXSID90160647

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 143 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.21e-01

Confidence level: 5.52e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl phthalyl ethyl glycolate</div> <div>Measured: 347</div> <div>Predicted: 319</div>	<div>Image not found</div> <div>Crotoxypfos</div> <div>Measured: 100</div> <div>Predicted: 123</div>	<div>Image not found</div> <div>Imazapyr</div> <div>Measured: 100</div> <div>Predicted: 65.8</div>
<div>Image not found</div> <div>Imazethapyr</div> <div>Measured: 7.08</div> <div>Predicted: 77.7</div>	<div>Image not found</div> <div>Thiophanate-methyl</div> <div>Measured: 1780</div> <div>Predicted: 864</div>	